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The Study of Ferromagnetism in Manganese-Doped Zinc Telluride (Mn-doped ZnTe) Diluted Magnetic Semiconductor

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**THE STUDY OF FERROMAGNETISM IN MANGANESE-DOPED ZINC
TELLURIDE (Mn-doped ZnTe) DILUTED MAGNETIC SEMICONDUCTOR**



**A GRADUATE PROJECT SUBMITTED TO THE DEPARTMENT OF
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In PHYSICS

BY

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**December, 2022
BAHIR DAR, ETHIOPIA**

BAHIR DAR UNIVERSITY

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Abbreviations

DMS Diluted Magnetic Semiconductor

ZnMnTe Zinc Manganese Telluride

Mn Manganese

TV Television

FM Ferromagnetism

AFM Antiferromagnetism

M-RAM Magneto Resistive Random Access Memory

T Temperature

T_c Curie temperature

MS Magnetic Semiconductor

FET Field Effect Transistor

LED Light Emitting Diode

TM Transition Metal

ZnTe Zinc Telluride

RT Room Temperature

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Abstract

A spintronics device is multifunctional device, which allows the interplay between charge carriers and spin in a single system. These materials are very important in modern technology for non-volatility, fast data processing, low power consumption and high integration density. To achieve the advantages of a spintronics device, semiconductor materials are doped with magnetic impurity of transition metals to give diluted magnetic semiconductors which have both ferromagnetic and semiconductor properties. The main objective of this project is to study the ferromagnetism in Mn-doped ZnTe diluted magnetic semiconductors (DMSs). ZnTe when doped with a very low percent of Mn ion can exhibit room temperature ferromagnetism. Due to their ferromagnetic properties they can be used in spintronic applications. ZnMnTe systems with wurtzite structure and room temperature ferromagnetism are investigated using Heisenberg model Hamiltonian. The Hamiltonian includes exchange interactions with the nearest neighbors. Different calculations are performed using Holstein-Primakoff transformation and Green function formalism. The researches of the study reveal that the total average number of magnons and reduced magnetization are determined. In addition to this concentration dependent transition temperature and specific heat capacity of magnon are also predicted. The average number of magnon depends on temperature with $\langle n \rangle \sim T^{3/2}$ relation, specific heat capacity of magnon also depends on temperature with $C^{mag} \sim T^{3/2}$ relation, reduced magnetization decreases with increasing temperature and the transition temperature linearly depends on manganese concentration ion.

Key words: Semiconductor, Magnetism, DMS, Ferromagnetism, Spintronics,

Chapter one

Introduction

1. Back ground of the study

Semiconductors are materials which have property between conductors and insulators. Semiconductors can be elemental or compound. Compound semiconductors are important semiconductors than elemental semiconductors in spintronic devices. In addition to binary compound semiconductors, ternary compounds are made for special applications [1]. Recently, there has been growing interest in the Mn-based II-VI compound diluted magnetic semiconductor (DMS) nanostructures. This interest is stimulated by the possible realization of high performance optoelectronic devices due to the wide direct band gap and magnetic, magneto-electronic and magneto-optical properties for spintronics applications. Mn^{2+} acts as a paramagnetic center ($S = 5/2$) and sp-d exchange interaction occurs between the electron/hole band states of the semiconductors and the $Mn^{2+} 3d^5$ electron states in the DMS nanocrystals[2]. However, the fact that Mn is actually embedded inside the semiconductor unit cell is important for obtaining high-quality Mn-doped II-VI DMS nanomaterials [3]. Although Mn^{2+} ions can be incorporated thermodynamically up to their solid solubility limit (~50%), Mn has a tendency to be expelled from the semiconductor nanocrystal surface [4]. Zinc telluride (ZnTe) is an intrinsic wide-gap semiconductor material with a band gap of 2.23-2.26 eV, having a cubic crystal structure with a wide range of practical applications. Because of the possibility of hole-induced ferromagnetism and magneto-electronics applications, $Zn_{1-x}Mn_xTe$ single crystals, thin films, and quantum dots were extensively researched over the years[5]. Doping magnetic impurity such as Mn, in to this compound gives rise to DMS with both magnetic and semiconducting properties under certain critical temperature. Semiconductors work by exploiting the electric charge attached to electrons. But electrons in solids have another fundamental property known as spin which makes them act like small magnets. Computer hard discs, which consist of layers of metals such as cobalt and copper, already tap this magnetic property to produce memory storage. Semiconductor-based magnetic memories would enable computers to be like a TV set where it has not reloaded the operating systems. Achieving

spintronic devices to such kind is a step towards new breed of computer chips that will couple memory with information processing and photonic capabilities [6]. Such chips will retain data even when the computer is turned off, eliminating the consuming process of booting up information from hard drive to process [7]. Besides, eliminating long boot-up time M-RAM chips are likely to require far less power because controlling the current flow by altering electronic spin may require only small voltages. It could significantly extend battery life in hand-held electronic devices such as mobile phones. In addition, spin-based lasers and other light emitters could transmit data that is encoded or labeled by the polarization of light.

The current project work is intended to study ferromagnetism in Mn-doped ZnTe DMS. Ferromagnetism was studied mediating charge carriers where the interaction is attributed to the RKKY type as explained by the Dietl model [2]. This is one of the mechanisms suggested that could enhance ferromagnetism of localized Mn spin doped in to semiconductor ZnTe. Magnetic semiconductors (MS) are materials that exhibit both magnetic and semiconducting properties. MS is key to the development of spintronic devices such as nonvolatile memories, spin valve transistors, optical switches, spin-FETs and spin-LEDs [8]. Using ferromagnetic DMS such as Mn-doped ZnTe DMS in the field of spintronics (spin transport electronics), have different advantages such as non-volatility, increased data processing speed, decreased electric power consumption and increased integration densities.

Therefore, study of ferromagnetic diluted magnetic semiconductor is very significant because of ferromagnetic DMS have spin and charge electrons that possess potential applications in high temperature ferromagnetic spintronic and quantum computing devices. Mn-doped ZnO DMS is ferromagnetic DMS which is multifunctional material with co-existing of magnetic, semiconducting and optical properties.

1.1. Statement of the Problem

Semiconductors are materials which have semiconducting properties. These materials are important for charge dependent electronic devices. The electronic devices which are building from these materials are passive to process in spintronics devices due to absence of spin dependent properties. Magnetic materials have their own advantages in electronic devices but such materials do not process actively in modern technology of spintronics devices due to the absence of charge dependent properties. Combining the semiconductor and magnetic properties of materials give better application in spintronics devices, such materials are ferromagnetic DMS. There are natural ferromagnetic materials which are applicable in modern spintronic devices but they are scarce. To overcome such problems, we should obtain ferromagnetic DMSs which combine the properties of magnetic and semiconducting properties which are applicable for modern technology. This is done by doping transition metals on compound semiconductors which give diluted magnetic semiconductors. DMSs are the most interesting magnetic semiconductor materials in spintronic devices. The room temperature ferromagnetism in these materials is the most problem in solid state physics. There are recently studied researches based on the transitional metal like Mn doped semiconductors such as II-VI and III-V semiconductors. But these DMSs are ferromagnetic materials below room temperature or at low temperature such as (III,Mn)V and (II,Mn)V. Therefore, modern technology needs transitional metal doped DMS at high temperature or at room temperature. Ferromagnetism of Mn-doped ZnTe DMS was studied by Sharma et al., [9] experimentally and Dietl et al., [2] theoretically. But their studies don't explain about average number of magnons, magnon specific heat capacity and other quantities as a function of temperature in these systems. So, this motivated me to study ferromagnetism in Mn-doped ZnTe DMS based on Heisenberg model Hamiltonian using Green function formalism.

1.2 Project Objectives

1.2.1 General Objectives

The general objective of this project work is to study ferromagnetism in Mn-doped ZnTe diluted magnetic semiconductor.

1.2.2 Specific Objectives

The specific objectives of the study are:

- To determine the relation between magnetization and temperature of Mn-doped ZnTe DMS.
- To calculate the ferromagnetic transition temperature of Mn-doped ZnTe DMS.
- To calculate heat capacity of ferromagnetic Mn-doped ZnTe DMS.
- To determine average number of magnons for Mn-doped ZnTe DMS.

1.3. Research questions

The research questions to be answered by this study include:

1. What relation exists between magnetization and temperature of Mn-doped ZnTe DMS?
2. What factors affect the ferromagnetic transition temperature of Mn-doped ZnTe DMS?
3. How is the heat capacity of ferromagnetic Mn-doped ZnTe DMS expressed?
4. What is the mathematical expression for the average number of magnons in Mn-doped ZnTe DMS?

1.4. Organization of the project

The project comprises five chapters. Chapter one covers a brief introduction of the project work. Chapter two presents reviews of theoretical and experimental works which are closely related to our project work. Mathematical techniques used in this work are briefly described in chapter three. In chapter four, results and discussions of the project work are presented. Finally, in chapter 5, conclusions and recommendations of the project are presented.

Chapter Two

2. Literature Review

2.1 Introduction

A newly emerging interest in the field of manipulating charge and spin of electrons in spintronics has been enhancing the study of magnetic impurity and semiconductor alloys. Such systems can be magnetic semiconductors (intrinsically) and diluted magnetic semiconductors (doped) [10]. Magnetic semiconductors are materials possessing magnetic and semiconducting properties intrinsically such as rare-earth chalcogenides in which Europium chalcogenides are widely studied [11] and Cr-spinels which are families of important AB_2X_4 oxide minerals, where A and B are metal ions and $X = O, S, Se, Te$. Chromium spinel oxides, ACr_2O_4 , offer the opportunity to study magnetic frustration in the absence of charge and orbital effects. Researches on europium chalcogenides EuX , with $X = O, S, Se, Te$ have been the subject of many studies for several years. The identification of EuO by Matthias et al. In 1961 [11], which was reported as truly ferromagnetic at 77K which is the first rare earth oxide found to be ferromagnetic with true ferromagnetic coupling. This is the first motivation for further investigations of europium chalcogenides as magneto-optic memories in computers and magneto-optic modulators [12]. However, the study on such magnetic semiconductor systems is ceased due to the complexity during the crystal growth while controlling magnetic spins and charges separately making the production of mono-crystalline europium chalcogenides on the industrial scale which is very expensive also.

At present, it is commonly accepted that there is no chance for any industrial application of these compounds and the current interest in the use of magnetic semiconductors as light beam addressable memory system is focused on mixed valence systems [12] known as diluted magnetic semiconductors.

Diluted magnetic semiconductors (DMSs) are composed of host semiconductor doped with both localized spins and carries (electrons or holes). These doped materials are called diluted magnetic semiconductors (DMSs), which are typically II-VI or III-V semiconductors in which a

small fraction of their cations have been randomly substituted by magnetic ions such as transition metal ions. DMS based on II-VI semiconductors have been widely studied in the 80s. However these materials mainly present paramagnetic, spin glass or antiferromagnetic behaviors. The study of III-V DMS some years later led to the achievement of ferromagnetic compounds [13], but their low Curie temperature prevents them to use for application (i.e. at room temperature). Dietl et al proposed that based on the Zener model that the wide band gap semiconductor GaN and ZnO doped by manganese would be ferromagnetic with a Curie temperature exceeding room temperature. Requirements for functional MS are ferromagnetic properties at room temperature, possibly of n-type and p-type semiconducting behaviors and the ferromagnetic properties should be mediated by carriers. Additional advantages for the investigation of ZnO and GaN as DMSs are their optoelectronic properties of possible incorporation in existing semiconductor technology and encouragingly long spin coherence. The TiO₂ based DMS have also attracted much attention due to the achievement of room temperature ferromagnetism [2]. The ferromagnetic properties of DMSs result from a spin interaction between the electrons or holes in the sp bands of the semiconductor host and those of the localized d shells of the magnetic impurities. The collective interaction of atoms magnetic moment responsible for magnetic order can arise from indirect exchange interactions such as RKKY interaction (like in metals) or Zener mechanism. These are carriers mediated interactions over relatively large distances.

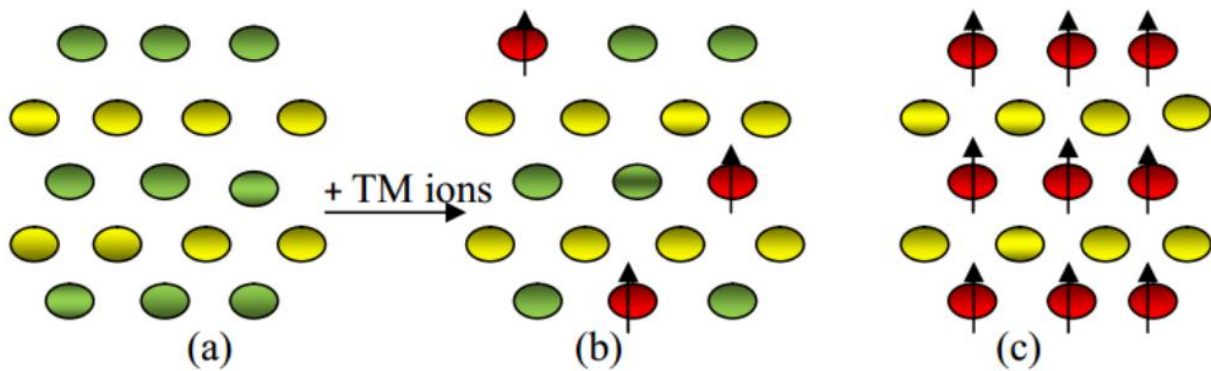


Figure 2.1 Illustration of (a) nonmagnetic semiconductor, (b) a DMS and (c) a MS [14].

2.2 The Magnetic Elements for Doping

The magnetic elements for doping purpose are mainly Cr, Mn and Fe from transition elements in forming diluted magnetic semiconductors [15]. In Mn^{+2} doped III-V based DMS, there is a valance mismatch between that of Mn and the group III elements with $S = 5/2$ creating holes in valance band and less soluble.

In Cr^{+2} doped III-V, the 3d electrons are less in number $4(1/2) = 2$ less magnetic impurity spins per atom result weak ordering in the compound. In Fe^{+2} the 3d electrons gives rise to $S = 4(1/2) = 2$ and Fe^{+3} gives the valance match with group III elements as Cr^{2+} in II-VI DMS. In II-VI semiconductors such as $ZnOMn^{+2}$ is more preferable for doping purpose due to the ionic radius of Mn and Zn is approximately same.

table2. 1Magnetic elements used for doping purpose in DMS [14]

Element	Cr^{24}	Mn^{25}	Fe^{26}	Cr^{+2}	Mn^{+2}	Fe^{+2}	Fe^{+3}
Configuration	$3d^5 4s^1$	$3d^5 4s^2$	$3d^6 4s^2$	$3d^4$	$3d^5$	$3d^6$	$3d^5$

2.3 Family of Diluted Magnetic Semiconductors

Semiconductor devices have become an integral part of our lives. Si is the prime elemental semiconductor that has revolutionized the microelectronics industry. However, Si is an indirect band gap semiconductor and thus an inefficient light emitter/absorber. Optoelectronic devices involve interaction between photons and electrons. Direct band gap semiconductors that show strong absorption/emission characteristics are best suited for such applications. Most widely used

semiconductors for optoelectronic device applications are compounds formed between elements of group II-VI and III-V of the periodic table.

2.3.1 II-VI based Diluted Magnetic Semiconductors

The II-VI DMS are based on semiconductors of group II elements and a group VI element (such as CdTe or ZnSe). In the II-VI DMS, some of the divalent sites (Cd/Zn) are substituted by a magnetic element typically Mn. This is because such +2 Mn ions are easily incorporated into the host II-VI crystals by replacing group II cations. Mn is also a group II element but in addition it has a half-filled 3d shell with a total spin $S = 5/2$. In the absence of other types of dopants, the $\text{II}_{1-x}\text{Mn}_x\text{VI}$ (where x is the fractional Mn concentration) is an insulator which exhibits dominantly antiferromagnetic (AFM) tendencies at low temperature [16] which results in the paramagnetic, antiferromagnetic or spins glass behavior of the material. The origin of this AFM tendency is expected antiferromagnetic exchange between the Mn spins. However, for low doping concentration x , the average distance between Mn spins is larger and this AFM direct exchange is rather small. When a low density of dopants is introduced in the system, each of them binds a hole (or electrons). For Mn spins which are very close to one another the direct antiferromagnetic (AFM) exchange is the dominant interaction. For fairly far apart Mn spins, the dominant magnetic interaction is the exchange between the charge carrier spins and the Mn spins.

2.3.2 III-V based Diluted Magnetic Semiconductors

An approach compatible with the semiconductors used in present day electronics is to make nonmagnetic III-V semiconductors, magnetic and even ferromagnetic by introducing a high concentration of magnetic ions. The III-V semiconductors such as GaAs are already in use in a wide variety of electronic equipment in the form of electronic and optoelectronics devices including cellular phones (microwave transistors), compact disks (semiconductor lasers) and in many other applications. Therefore, the introduction of magnetic III-V semiconductors opens up the possibility of using a variety of magnetic phenomena not present in conventional nonmagnetic III-V semiconductors used in the optical and electronics devices already established. When Mn is grown in a III-V semiconductor such as GaAs, the major difference with respect to the II-VI DMS is that the Mn atom provides both the $S = 5/2$ spin and the dopant charge carrier

(a hole since divalent Mn substitutes for trivalent Ga). As in the doped (II,Mn)VI systems, the main magnetic interactions in the (III,Mn)V DMS is the exchange between the Mn spins and the hole spins which is known to be AFM. This interaction is again proportional to the probability of finding the charge carrier at the Mn site [16]. III-V materials are among the most widely used semiconductors but the ferromagnetism of this material shows at low temperature[17].

2.3.3 Zinc Telluride Diluted Magnetic Semiconductors

As a host semiconductor, ZnTe, with a direct band gap of 2.26 eV, is considered to have great potential in thermoelectric and optoelectronic applications. In the last decade, ZnTe doped with transition metals, such as Mn, Cr, Cd and V, have attracted considerable attention owing to their interesting magnetic properties, fluorescence and structural compatibility with II–VI semiconductors and some important III–V semiconductors such as GaAs. In 2010, Mn-doped ZnTe was suggested to be a spin gapless semiconductor because of its theoretical band structure [18]. Therefore, it has potential for use as a spintronic material, motivating studies of its magnetic properties. Molecular beam epitaxy, high-temperature solid state reaction and vapor phase growth have been used to prepare Mn-doped ZnTe. The hydrothermal method is a more convenient approach that does not require a high temperature or a high vacuum. The method can easily produce a high-pressure environment that accelerates the chemical reactions, so it can be used to prepare many materials with multifunctional properties and interesting morphologies. However, to the best of our knowledge, difficulties in controlling the composition of the required multi-component system have prevented the use of the hydrothermal method in fabricating Mn-doped ZnTe. This work reports on a hydrothermal method for synthesizing nanoparticles of ZnTe doped with 3 at. % Mn [19, 20].

2.3.3 Ferromagnetism

Ferromagnetic materials have a spontaneous magnetization in the absence of the external field and manifest very large and permanent magnetization. Permanent magnetic moments in these materials result from atomic magnetic moments due to uncancelled electron spins. In a

ferromagnetic material, coupling interaction causes net spin magnetic moments of adjacent atoms to align to one another, even in the absence of an external magnetic field.

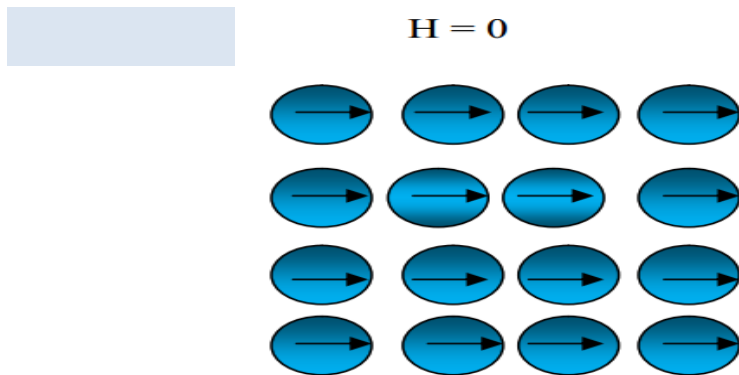


Figure 2.2 Schematic representation of spin alignment in a ferromagnetic material [14].

2.3.4 Spin glass

A spin glass is a disordered magnetic state. Spin glasses are the type of random magnets in which both ferromagnetic and antiferromagnetic interactions coexist, giving rise to the effects of randomness. An important characteristic of the spin glass state is that it accompanies a thermodynamic phase transition, usually being of second order from the high temperature paramagnetic state. The existence of such a thermodynamic spin glass transition and a thermodynamic spin glass phase makes the study of spin glasses appealing, since it implies the existence of a new magnetic state of matter distinct from the standard ferromagnets, antiferromagnets and their analogs. Spin glass forms an important family of magnetism along with other types of magnets.

2.4 Zinc Telluride (ZnTe)

Zinc telluride (ZnTe) is an intrinsic wide-gap semiconductor material with a band gap of 2.23-2.25 eV, having a cubic crystal structure with a wide range of practical applications. Because of the possibility of hole-induced ferromagnetism and magneto-electronics applications, $Zn_{1-x}Mn_xTe$ single crystals, thin films, and quantum dots were extensively researched over many years. However, future applications related to high-density magnetic recording and waveguide-type

optical communications require a fine control of the materials at the nanoscale level, and organization of the spintronic materials into two- dimensional (2D) or three dimensional (3D) architectures on a microscopic chip(Turner et al., 1988) [21]. ZnTe is a very low cost and easily available material. Moreover, there are no environmental hazards associated with this material due to its non-toxic nature.

2.4.1 Crystal structure of ZnTe

Zinc telluride is a binary chemical compound with the formula ZnTe. This solid semiconductor material with a direct band gap of 2.26 eV. It is usually a p type semiconductor. Its crystal structure is cubic, like that for sphalerite and diamond.

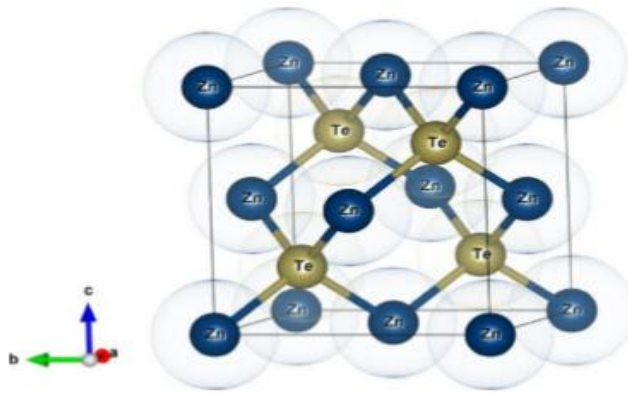


Figure 2.3 representation of ZnTe crystal structure[22]

2.5 Mn-doped ZnTe DMS

In Mn-doped ZnTe DMS a small portion of atoms is randomly substituted by Mn elements giving rise to localized magnetic moments in the ZnTe semiconductor. The presence of magnetic ion affects the free carrier behavior through the sp-d exchange interaction between the localized magnetic moments and the spins of the charge carrier's [23]. Mn elements have valence electrons corresponding to the 4s orbital and have partially filled 3d shells, i.e. Mn with the shell structure of $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^2$. ZnTe is wurtzite structure which is formed by tetrahedral (s-p3) bonding. Generally, Mn ions substitute for the cations of the host semiconductors i.e., Zn sites in ZnTe. In ZnTe the Mn contributes its 4s2 electrons to the s-p3 bonding and can therefore, substitutionally replace the Zn in the tetrahedral bonding to form a TM^{2+} charge state. The 3d band of the Mn^{2+} ion is exactly half-filled with 5 electrons among the 10 available states with an energy gap between the up-spin (\uparrow) occupied states and empty down-spin (\downarrow) states. The d bands of Mn hybridize with the host valence bands (O bands in ZnTe) and form the tetrahedral bonding. This

hybridization gives rise to the exchange interaction between the localized 3d spins and the carriers in the host valence band.

2.6 Ferromagnetism in Mn-doped ZnTe DMS

ZnTe based DMSs are potential candidates for RT ferromagnetism predicted first time by Dietl and co-workers (Dietl et al., 2000) [2]. Pure ZnTe is diamagnetic in nature [24]. Doped ZnTe semiconductor can show ferromagnetism. The occurrence of ferromagnetism in DMSs has been long debated due to confronting reports. Considerable doubts have been expressed Mn clusters are expected to give an antiferromagnetic state rather than a ferromagnetic (FM) order; very small clusters can be ferromagnetic [2]. The ionic radius of Mn^{2+} is similar to Zn^{2+} which means that Mn^{2+} ion can substitute the Zn^{2+} ion [25]. The first reports of room temperature FM ordering in Mn-doped powder, bulk pellets as well as thin films with Curie temperature above 300K comes from Sharma et al [9]. This was confirmed by Blythe et al [26] who made a detailed study of the dependence of the FM ordering on the processing temperature. On the contrary, Kane et al [27] claimed no evidence of an FM ordering in $Zn_{1-x}Mn_xTe$, $Zn_{1-x}Co_xO$ bulk single crystals. Kittilstved et al [28] have on the other hand not only observed high Tc ferromagnetism in ZnMnTe and ZnCoO systems but also show their Tc can be manipulated. Various theoretical attempts have been put forward to explain the ferromagnetism in these DMS systems. In ZnTe system it has been proposed that the ferromagnetism can be obtained by the mediation of the shallow donors or acceptors [28] or the holes in the valence band. Undoped ZnTe shows a diamagnetic behavior while Mn doped ZnTe shows ferromagnetic behavior. This indicates that the ferromagnetism for Mn doped ZnTe comes from the presence of Mn ions in the ZnTe host matrix. This study also showed that the increased concentration of Mn will produce antiferromagnetic behavior which comes from the super exchange of the Mn-Mn interaction [29].

2.7 Spintronic Materials and Devices

Spintronics is a branch of electronics emerged from the diluted magnetic semiconductors in aspect of utilization of the spin in addition to the charge of the carrier in semiconductor [30]. There are two main categories of spintronic devices passive and active. Passive spintronics devices make use of spin degrees of freedom. The net polarization of spins in a material is used for data storage. Active spintronic devices employ both the spin and charge degrees of freedom which depend on manipulation to generate important devices with the capability of both traditional electronics and passive spintronics. Spin is an intrinsic quantum property of electrons and is closely related to magnetism. In many materials electron spins are equally present in both up and down state and no transport properties are dependent on spin. Therefore, spintronic devices require generation or manipulation of spin polarized population of electrons results excess of spin up or down electrons. In traditional electronics the electron spins are randomly oriented and have no effect on operation

and performance of a device but spintronics device is that the currents are spin polarized and the spin is used to control current flow or store data.

Spintronics devices are smaller than 100 nm in size (make it smaller, make it better), large storage capacity per volume, faster operations and less dissipation [31]. Spintronics is closely linked with the advantage of nanotechnology and spin dependent phenomena in transport. DMS materials play an important role in developing peculiar spintronic devices having charge and spin of electrons for information processing [32]. The main goal of spintronics is to gain knowledge on spin dependent phenomena and to exploit them for new functionalities. The advantages of spin over charge are that spin can be easily manipulated by externally applied magnetic field, a property already in use in magnetic storage technology [30]. Potentially significant property of spin is its long coherence or relaxation time once created it tends to stay that way for a long time but charge states are easily destroyed by scattering or collision with defects, impurities or other changes. Already the spintronics plates are used in the field of mass storage devices and have led to compressing massive amounts of data into a small area. Generally, the spintronics offers a variety of potential improvements that include non-volatility, high switching speed, high energy efficiency and the ability to be customized and reconfigured [33].

2.8 Exchange Interaction

The interactions among electrons allow the spins or magnetic moments to communicate in a material. This induces a long range ordering to make materials unique. The simplest type of exchange interactions among electrons are the dipole-dipole interactions. The exchange interactions are considered as electrostatic interactions, arising due to the change in energy with the change of distance between charges of the same sign. The exchange interactions create the stability among electrostatic and magnetostatic energies. Spin-spin interaction plays important role in formation of different magnetic moments. These interactions demonstrate the behavior of long range order of unpaired electrons called exchange interactions. Some types of exchange interactions are:

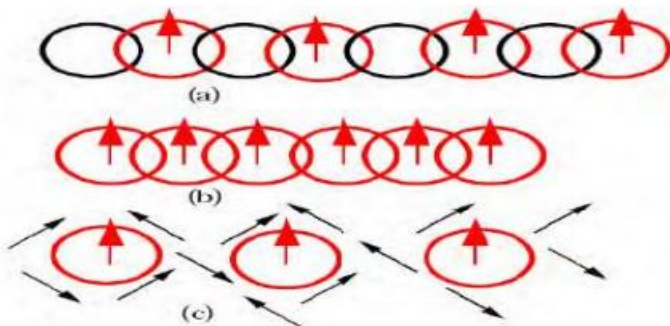


Figure 2.1 illustration of (a) super exchange (b) direct exchange and (c) indirect exchange[34].

Direct exchange Interaction: it arises from the direct coulomb interaction among electrons from the two ions [35]. Mostly, these interactions are not considered essential to control magnetic properties due to the direct overlap of the electronic wave functions of two nearest neighboring or adjacent magnetic atoms.

Super exchange Interaction: is interaction between the magnetic impurities which is mediated by nonmagnetic atoms. This exchange interaction is long ranged interaction. For II-VI DMSs the super exchange, resulting from the sp-d hybridization is by far the dominant spin-spin interaction because modulatedly undoped such DMSs have no free carriers to mediate the interaction.

Indirect exchange Interaction: Exchange interaction mediated by free electrons. The localized moments spin polarizes the conductive electrons. This spin polarization then combines with the localized adjacent magnetic moments. These exchange interactions are indirect because no direct coupling is involved between magnetic moments. These exchange interactions can arise through some other mechanisms such as Zener model or RKKY (Ruderman Kittel Kussaya Yoshida) interactions. These interaction mechanisms involve in DMSs like compounds.

2.9 Theoretical approach to express DMS

The ferromagnetism in diluted magnetic semiconductors can be described using different models theoretically. Different models express different properties of DMS.

Zener exchange model: This model is also Zener mean field model. In this model, exchange interactions lead to the ferromagnetic coupling due to the free holes mediating between TM atoms. This exchange model was proposed by Zener. In semiconductors, average distance among charge carriers is typically much greater than the spins. In this case, exchange interactions through these intermediate carriers are usually ferromagnetic which are associated with most of spin pairs (Schwabe et al., 1996) [36].

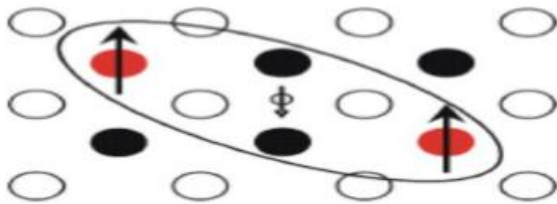


Figure 2.2 Ferromagnetic coupling of localized TM spins through the free holes [36].

RKKY interaction model: The RKKY interaction model (Yosida, 1996) [37] explains the magnetic interaction among delocalized conduction electrons and a single localized magnetic ion. The conduction electron lying near to the magnetic ion in structure is magnetized and operates as a

field to affect the polarization of neighboring magnetic ions with an oscillatory manner. These oscillations mediate either anti-ferromagnetic or ferromagnetic coupling which depends upon the distance between these magnetic ions. The RKKY model is very efficient when high density of delocalized electrons presents in structure. These are indirect exchange interactions with much longer range than super exchange interactions.

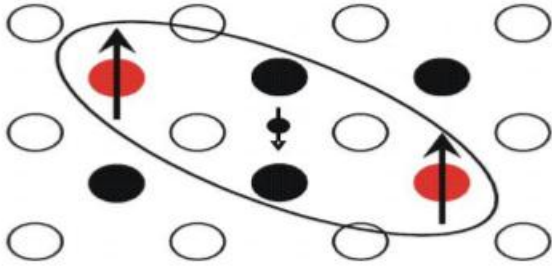


Figure 2.3 RKKY model describes the mediation of conduction electrons between magnetic atoms[37].

This mechanism was first proposed by Ruderman and Kittel through hyperfine interactions caused by the coupling of nuclear magnetic moment and conduction electrons. Kasuya and Yoshida then extended this model to introduce these interactions known as RKKY interactions. When an impurity of magnetic element is located in the structure of a compound, spin of conduction electron is dictated by the spin of impurity. Spin polarization of conduction electrons as a result produced concentric rings of localized spins around the impurity. RKKY interactions, hence, coupled through spin coupling of charge carriers due to indirect interactions among distant magnetic impurities (Fukuma et al., 2008) [38]. In this work we have used indirect exchange interaction. The model which we have used in this work is RKKY model because it is model which works at a distance due to indirect interactions.

Chapter Three

3. Mathematical Techniques for spin waves in DMS

3.1 Formulation of the problem

In magnetic phenomena of solid materials electrons are important particles due to its spin and the associated magnetic moment. For theoretical description of spin waves of DMS, the model of dopant spin exchange mediated by holes is used. The Heisenberg model Hamiltonian or a magnetic interaction of the Heisenberg model type which expresses the exchange interaction between spins is

$$H = -2 \sum_{ij} J_{ij} S_i \cdot S_j \quad (3.1)$$

Where J_{ij} is known as the exchange coupling constant between spin i and spin j , it is positive if the interaction is ferromagnetic and negative if it is antiferromagnetic [39].

A model Hamiltonian which is useful in understanding the properties of spin wave in ferromagnetic such as Mn-doped ZnTe DMS is Heisenberg model Hamiltonian. In this model the atoms or ions are arranged in a regular lattice position and each of them carries total spin S and a magnetic moment $g\mu_B S$, where μ_B is the Bohr magneton and g is the Land's g -factor. The Hamiltonian with external magnetic field is written as [40]

$$H = -J \sum_{ij} S_i \cdot S_j - 2\mu_B H_{ex} \sum_i S_i^z \quad (3.2)$$

Where H_{ex} an external magnetic field along z -direction, J is the measure of the exchange interaction. In ferromagnetic DMSs, the ground state is one in which all the spins are aligned in the direction of external magnetic field [41]. An approximate description of this system in terms of elementary excitations is possible through a transformation originally suggested by Holstein and Primakoff [42]. On the ferromagnetic Heisenberg Hamiltonian equation (3.2) only nearest neighbor's interaction is considered. Assuming here i and j refer to nearest neighbor lattice sites,

$S_i \cdot S_j$ is called an exchange interaction and the coefficient J_{ij} is called exchange constant (i.e $J_{ij} = J$)

where J is constant and S_i, S_j are operators which have spin components. Although each atom has three components of each spin vector only two of the components are independent.

$$S_i = S_i^x + S_i^y + S_i^z \quad (3.3)$$

$$S_j = S_j^x + S_j^y + S_j^z \quad (3.4)$$

Where i and j are site of atoms.

Using the rule of dot product of vectors, $A \cdot B = A_x B_x + A_y B_y + A_z B_z$

$$H = -J_{ij} \sum_{ij} S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z - 2\mu_B H_{ex} \sum_i S_i^z \quad (3.5)$$

$$\text{where } S_i^x = \frac{1}{2}(S_i^+ + S_i^-), S_j^x = \frac{1}{2}(S_j^+ + S_j^-) \text{ and } S_i^z = S - \alpha_i^+ \alpha_i \quad (3.6)$$

where $\alpha_i^+ \alpha_i$ is number operator for bosons and $S_i^+(S_i^-)$ are raising(lowering) spin operators for site i .

$$S_i^y = \frac{1}{2i}(S_i^+ - S_i^-), S_j^y = \frac{1}{2i}(S_j^+ - S_j^-) \text{ and } S_j^z = S - \alpha_j^+ \alpha_j \quad (3.7)$$

$$S_i^x S_j^x = \frac{1}{4} [S_i^+ S_j^+ + S_i^+ S_j^- + S_i^- S_j^+ + S_i^- S_j^-] \quad (3.8)$$

$$S_i^y S_j^y = \frac{1}{4} [-S_i^+ S_j^+ + S_i^+ S_j^- + S_i^- S_j^+ - S_i^- S_j^-] \quad (3.9)$$

$$S_i^z S_j^z = S^2 - S \alpha_j^+ \alpha_j - S \alpha_i^+ \alpha_i + \alpha_i^+ \alpha_i \alpha_j^+ \alpha_j \quad (3.10)$$

Rewriting the Hamiltonian in terms of the raising and lowering spin operators:

$$H = \sum_{ij} -J_{ij} \left[\frac{1}{2} [S_i^+ S_j^- + S_i^- S_j^+] + S^2 - S \alpha_j^+ \alpha_j - S \alpha_i^+ \alpha_i + \alpha_i^+ \alpha_i \alpha_j^+ \alpha_j \right] - 2\mu_B H_{ex} \sum_i S_i^z \quad (3.11)$$

where $S_i^- S_j^+$ creates or destroy spin deviation on i and j sites and $S_i^+ S_j^-$ is exchange spin deviation between two sites i and j.

$$H = \sum_{ij} -J_{ij} \left[\frac{1}{2} [S_i^+ S_j^- + S_i^- S_j^+] + S^2 - S \alpha_j^+ \alpha_j - S \alpha_i^+ \alpha_i \right] - 2\mu_B H_{ex} \sum_i S_i^z \quad (3.12)$$

The term order $\alpha_i^+ \alpha_i \alpha_j^+ \alpha_j$ is ignored, because it represents higher order scattering of spin waves which are unimportant at low temperatures.

Using the spin operators in terms of creation and annihilation operators, we can rewrite the spin operators in the Heisenberg model Hamiltonian in terms of boson operators using the Holstein-Primakoff (H.P) transformation which is very useful for studying magnetically ordered state and their excitations [41]. The H.P transformation expressed spin raising and lowering operators on sites i and j in terms of boson creation and annihilation operators considering impurity concentration x is given by,

$$S_i^+ = (\sqrt{2xS - a_i^+ a_i}) a_i = (2xS)^{1/2} \left(1 - \frac{a_i^+ a_i}{2xS} \right)^{1/2} a_i \quad (3.13)$$

$$S_i^- = a_i^+ (\sqrt{2xS - a_i^+ a_i}) = (2xS)^{1/2} a_i^+ \left(1 - \frac{a_i^+ a_i}{2xS} \right)^{1/2} \quad (3.14)$$

$$S_i^z = xS - a_i^+ a_i \quad (3.15)$$

where $\alpha_i^+ \alpha_i$ and $\alpha_j^+ \alpha_j$ are the number operators for sites i and j, i.e., they count the number of bosons on i and j sites respectively. The α_i^+ and α_j^+ creates spin deviations at sites i and j respectively. Using the Taylor series given by,

$$f(X) = f(0) + \frac{f'(0)X}{1!} + \frac{f''(0)X^2}{2!} + \dots \quad (3.16)$$

$$\text{Let } X = \frac{\alpha_i^+ \alpha_i}{2xS} \quad \text{and } f(x) = (1-x)^{1/2}$$

$$f(0) = 1, \dot{f}(x) = -\frac{1}{2}(1-x)^{-1/2}, \quad \ddot{f}(x) = -\frac{1}{4}(1-x)^{-3/2} \quad (3.17)$$

equation(3.16) becomes,

$$f(X) = 1 - \frac{X}{2} - \frac{X^2}{8} + \dots \quad (3.18)$$

Using equation(3.18), we can rewrite equation(3.13) and equation(3.14) as follows

$$S_i^+ = (2xS)^{1/2} \left(1 - \frac{\alpha_i^+ \alpha_i}{4xS} - \frac{(\alpha_i^+ \alpha_i)^2}{32x^2 S^2} + \dots \right)^{1/2} \alpha_i \quad (3.19)$$

$$S_i^- = (2xS)^{1/2} \left(1 - \frac{\alpha_i^+ \alpha_i}{4xS} - \frac{(\alpha_i^+ \alpha_i)^2}{32x^2 S^2} + \dots \right)^{1/2} \alpha_i^+ \quad (3.20)$$

This implies that the relation between the S and α in i and j sites can be approximated by

$$S_i^+ = (2xS)^{1/2} \alpha_i \quad S_j^+ = (2xS)^{1/2} \alpha_j \quad (3.21)$$

$$S_i^- = (2xS)^{1/2} \alpha_i^+ \quad S_j^- = (2xS)^{1/2} \alpha_j^+ \quad (3.22)$$

The higher order terms $\alpha_i^\dagger \alpha_i$, $\alpha_i^\dagger \alpha_i \alpha_i^\dagger \alpha_i$ and $\alpha_i^\dagger \alpha_i \alpha_j^\dagger \alpha_j$ are ignored due to scattering. By substituting equation.(3.21) and (3.22) in to equation.(3.12), the result is

$$H = \sum_{ij} -J_{ij} \chi S [\alpha_i \alpha_j^\dagger + \alpha_i^\dagger \alpha_j + S - \alpha_j^\dagger \alpha_j - \alpha_i^\dagger \alpha_i] - 2\mu_B H_{ex} N \chi S + 2\mu_B H_{ex} \sum_i \alpha_i^\dagger \alpha_i \quad (3.23)$$

$$H = \sum_{ij} -J_{ij} \chi S^2 - 2\mu_B H_{ex} N \chi S + \sum_{ij} -J_{ij} \chi S [\alpha_i \alpha_j^\dagger + \alpha_i^\dagger \alpha_j - \alpha_j^\dagger \alpha_j - \alpha_i^\dagger \alpha_i] + 2\mu_B H_{ex} \sum_i \alpha_i^\dagger \alpha_i \quad (3.24)$$

$$H = H_o + H^{magnon} \quad (3.25)$$

Taking the magnon part of the relation, we have

$$H^{magnon} = \sum_{ij} -J_{ij} \chi S [\alpha_i \alpha_j^\dagger + \alpha_i^\dagger \alpha_j - \alpha_j^\dagger \alpha_j - \alpha_i^\dagger \alpha_i] + 2\mu_B H_{ex} \sum_i \alpha_i^\dagger \alpha_i \quad (3.26)$$

The terms in the square bracket are operators expressing explicitly the handing of spin deviations from one site to the next. Since the spin deviations are not localized to particular lattice site but propagate throughout, we need the creation operators that create non-localized excitations through the sample. The transformation that will do this is Fourier transformation variables for boson operators, which are given by [43]

$$\alpha_i = \frac{1}{\sqrt{N}} \sum_k e^{-ik \cdot r_i} b_k \quad \text{and} \quad \alpha_i^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{ik \cdot r_i} b_k^\dagger \quad (3.27)$$

$$\alpha_j = \frac{1}{\sqrt{N}} \sum_k e^{-ik \cdot r_j} b_k \quad \text{and} \quad \alpha_j^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{ik \cdot r_j} b_k^\dagger \quad (3.28)$$

where k is magnon wave vector, b_k is magnon creation operator, b_k^\dagger is magnon annihilation operator, N is number of lattice and since we consider nearest neighbor interaction we can write

$r_j = r_i + \delta$, where δ is vector connecting nearest neighbor sites, r_j and r_i are electron coordinates. Spins locally deviate only by a small amount from their ground state values parallel to z-axis as spin wave is passed. The total number of magnons equals the total spin deviation quantum number.

The commutation relation b_k obey the same kind of commutation relation as the original boson operators α_j , i.e., $[b_k; b_{k'}^\dagger] = \delta_{kk'}$. So there are as many operators b_k as there are operators δ_j .

$$\begin{aligned}
H^{mag} = & -J\chi S \sum_{ij} \left[\frac{1}{\sqrt{N}} \sum_k e^{-ik \cdot r_i} b_k \cdot \frac{1}{\sqrt{N}} \sum_{k'} e^{ik' \cdot r_j} b_{k'}^\dagger + \frac{1}{\sqrt{N}} \sum_k e^{ik \cdot r_i} b_k^\dagger \cdot \frac{1}{\sqrt{N}} \sum_{k'} e^{-ik' \cdot r_j} b_{k'} - \right. \\
& \left. \frac{1}{\sqrt{N}} \sum_k e^{ik \cdot r_j} b_k^\dagger \cdot \frac{1}{\sqrt{N}} \sum_{k'} e^{-ik' \cdot r_j} b_{k'} - \frac{1}{\sqrt{N}} \sum_k e^{ik \cdot r_i} b_k^\dagger \cdot \frac{1}{\sqrt{N}} \sum_{k'} e^{-ik' \cdot r_i} b_{k'} \right] + \\
& 2\mu_B H_{ex} \sum_k \frac{1}{\sqrt{N}} \sum_k e^{ik \cdot r_i} b_k^\dagger \cdot \frac{1}{\sqrt{N}} \sum_{k'} e^{-ik' \cdot r_i} b_{k'}
\end{aligned}
\tag{3.29}$$

$$\begin{aligned}
H^{mag} = & \frac{-J\chi S}{N} \sum_{i\delta k, k'} \left[e^{-ik \cdot r_i} b_k e^{ik' \cdot (r_i + \delta)} b_{k'}^\dagger + e^{ik \cdot r_i} b_k^\dagger e^{-ik' \cdot (r_i + \delta)} b_{k'} - e^{ik \cdot (r_i + \delta)} b_k^\dagger e^{-ik' \cdot (r_i + \delta)} b_{k'} - \right. \\
& \left. e^{ik \cdot r_i} b_k^\dagger e^{-ik' \cdot r_i} b_{k'} \right] + \frac{1}{N} 2\mu_B H_{ex} \sum_{i k k'} e^{ik \cdot r_i} b_k^\dagger e^{-ik' \cdot r_i} b_{k'}
\end{aligned}
\tag{3.30}$$

$$\begin{aligned}
H^{mag} = & \frac{-J\chi S}{N} \sum_{i\delta k, k'} \left[e^{-i(k-k')r_i} e^{ik' \cdot \delta} b_k b_{k'}^\dagger + e^{i(k-k')r_i} e^{-ik' \cdot \delta} b_k^\dagger b_{k'} - e^{i(k-k')r_i} e^{i(k-k')\delta} b_k^\dagger b_{k'} - \right. \\
& \left. e^{i(k-k')r_i} b_k^\dagger b_{k'} \right] + \frac{1}{N} 2\mu_B H_{ex} \sum_{i k k'} e^{i(k-k')r_i} b_k^\dagger b_{k'}
\end{aligned}
\tag{3.31}$$

$$\text{By using } \sum_i e^{i(k-k')r_i} = N, \text{ for } k = k' \tag{1.32}$$

$$H^{mag} = \sum_k \left[-J\chi S \left(\sum_\delta e^{ik' \cdot \delta} b_k b_{k'}^\dagger + \sum_\delta e^{-ik' \cdot \delta} b_k^\dagger b_{k'} - b_k^\dagger b_{k'} - b_k^\dagger b_{k'} \right) + 2\mu_B H_{ex} b_k^\dagger b_{k'} \right] \tag{3.33}$$

using,

$$\gamma_k = \frac{1}{z} \sum_\delta e^{ik' \cdot \delta} \text{ and } \gamma_{-k} = \frac{1}{z} \sum_\delta e^{-ik' \cdot \delta} \tag{3.34}$$

are the magnon functions, which in the approximation depends only on the positions of the nearest neighbor spins.

$$H^{mag} = \sum_k [-JxSz(\gamma_k b_k b_{k'}^+ + \gamma_{-k} b_k^+ b_{k'}) - 2b_k^+ b_{k'}] + g\mu_B H_{ex} b_k^+ b_{k'} \quad (3.35)$$

$$H^{mag} = \sum_k [-JxSz(\gamma_k(1 + b_k^+ b_k^+) + \gamma_{-k} b_k^+ b_{k'} - 2b_k^+ b_{k'}) + g\mu_B H_{ex} b_k^+ b_{k'}] \quad (3.36)$$

$$H^{mag} = \sum_k [-JxSz(\gamma_k + \gamma_k b_k^+ b_k + \gamma_{-k} b_k^+ b_{k'} - 2b_k^+ b_{k'}) + g\mu_B H_{ex} b_k^+ b_{k'}] \quad (3.37)$$

$$H^{mag} = -JxSz \sum_k \gamma_k - \sum_k [JxSz(\gamma_k b_k^+ b_k + \gamma_{-k} b_k^+ b_{k'} - 2b_k^+ b_{k'}) + g\mu_B H_{ex} b_k^+ b_{k'}] \quad (3.38)$$

$$H^{mag} = -[JxSz \sum_k [2\gamma_k b_k b_{k'}^+ - 2b_k^+ b_{k'}] + g\mu_B H_{ex} \sum_k b_k^+ b_{k'}] \quad (3.39)$$

Noting that $\sum_k \gamma_k = 0$ and $\gamma_k = \gamma_{-k}$ if there is a center of symmetry.

$$H^{mag} = \sum_k [-2JxSz\gamma_{-k} + 2JxSz + g\mu_B H_{ex}] b_k^+ b_k \quad (3.40)$$

$$H^{mag} = \sum_k [2JxSz(1 - \gamma_{-k}) + g\mu_B H_{ex}] b_k^+ b_k \quad (3.41)$$

At low temperature spin waves are harmonic oscillator or phonon type Hamiltonian. Under this assumption, the magnon part of the Hamiltonian can be simply written as,

$$H = \sum_k \hbar \omega_k b_k^+ b_k \quad (\hbar = 1)$$

$$\text{where } \omega_k = 2JxSz(1 - \gamma_k) + g\mu_B H_{ex} \quad (3.42)$$

The equation(3.42) is the magnon dispersion where z is the nearest neighbor spins. Considering the case of simple cubic lattice in 3D, the nearest neighbors ($z = 6$) are along the $\pm X, \pm Y$ and $\pm Z$ axes at distance α and we have,

$$\gamma_k = \frac{1}{3}(\cos k_x \alpha + \cos k_y \alpha + \cos k_z \alpha) \quad (3.43)$$

From equation (3.42) above, $1 - \gamma_k$ is given by

$$1 - \gamma_k = 1 - \frac{\cos k_x \alpha + \cos k_y \alpha + \cos k_z \alpha}{3} = 1 - \cos k \alpha \quad (1.44)$$

where, $k_x + k_y + k_z = k$.

When $1 - \cos k \alpha$ expands, it becomes $\frac{k^2 \alpha^2}{2}$ and, for $k \alpha \ll 1$,

it becomes $\cong k^2 \alpha^2$.

Equation (3.42) becomes

$$\text{Hence } \omega_k = 2xJSzk^2 \alpha^2 + g\mu_B H_{ex} \quad (3.45)$$

$$\omega_k = Ak^2 + g\mu_B H_{ex} \quad (3.46)$$

where $A = 2xJSz\alpha^2$.

In this case ferromagnetic ordering is considered where the externally applied field is very small and negligible, so that H_{ex} is taken to be zero.

Thus, we get,

$$\omega_k = Ak^2 \quad (3.47)$$

Which implies $\omega_k \propto k^2$ (parabolic wave vector dispersion).

3.2 The Green Function Formalism

The Green functions play important role in the theoretical treatment of the many body propagators which are used to find the average behavior of one or two typical particles. So propagators are the basic quantities that describe the average behavior. There are different Green functions or propagators: One-particle, two-particles, n-particles, advanced, retarded and causal.

The propagator G yields directly the energies, life-time of the quasi-particles, momentum distribution, the spin, the particle density and used to calculate ground state energy [33]. The two-particle propagator G2 gives directly energy, the life-time of collective excitation, magnetic susceptibility and the electrical conductivity. The term “advanced” gives the state of the system at previous times based on the state of the system at the present time. The retarded one gives the present state of the system as it has evolved from the state at the previous times i.e., the effect of retardation [44]. The solution for the two Green function depends on boundary conditions: $G_r(t, t') = 0$ for $t < t'$ and $G_a(t, t') = 0$ for $t > t'$ and Green function is not defined for $t = t'$. The double-time temperature dependent Green functions are useful in calculating the average of dynamical quantities [45].

To calculate the Green's function $G(t, t')$ for the double-time temperature dependent, The Green function can be used the general equation of motion for Heisenberg operators $A(t)$ and $B(t')$. The retarded Green function $G_r(t, t')$ is given by,

$$G_r(t, t') \equiv \langle \langle A(t); B(t') \rangle \rangle_r = -i\theta(t - t') \langle [A(t), B(t')] \rangle_r$$

(3.48)

In equation (3.48), notations $\langle \langle \dots \rangle \rangle_r$ represents Green functions, single pointed bracket $\langle \dots \rangle$ represents the thermal average over a canonical ensemble, The square bracket $[\dots]$ denotes

commutator and anti-commutator, which is used in Fermionic system in Green function occurring in a certain problems. So, $A(t)$ and $B(t')$ are either Fermion or Boson operators and correspondingly the commutation, $[A(t), B(t')]_{\pm} = A(t)B(t') \pm B(t')A(t)$ [46] and $\theta(t - t')$ is the Haviside step

function having the property:

$$\theta(t - t') = \begin{cases} 1, & \text{for } t - t' > 0 \\ 0, & \text{for } t - t' < 0. \end{cases}$$

The Green functions will not depend on t and t' separately, but depend only on the difference $t - t'$.

Using boson operators b_k and b_k^+ , the Green function is expressed as,

$$G_{kk'}(t - t') = \langle \langle b_k(t), b_{k'}^+(t') \rangle \rangle = -i\theta(t - t') \langle [b_k(t), b_{k'}^+(t')] \rangle$$

$$(3.49)$$

To obtain the equation of motion we can multiply both sides equation (3.49) by i and differentiate it with respect to time (t).

$$i \frac{d}{dt} G_{kk'}(t - t') = i \frac{d}{dt} \langle \langle b_k(t); b_{k'}^+(t') \rangle \rangle = i \frac{d}{dt} \langle \langle b_k; b_{k'}^+ \rangle \rangle$$

$$i \frac{d}{dt} G_{kk'}(t - t') = \frac{d}{dt} \theta(t - t') \langle [b_k, b_{k'}^+] \rangle - i\theta(t - t') \langle \left[\frac{id}{dt} b_k; b_{k'}^+ \right] \rangle$$

$$(3.50)$$

$$\text{since, } \frac{d}{dt} \theta(t - t') = \delta(t - t') \text{ and } \frac{id}{dt} b_k = [b_k(t), H]$$

$$\frac{id}{dt} \langle\langle b_k; b_{k'}^+ \rangle\rangle = \delta(t - t') \langle\langle [b_k, b_{k'}^+] \rangle\rangle + \langle\langle [b_k, H]; b_{k'}^+ \rangle\rangle$$

(3.51)

Let $G_{kk'}(\omega)$ be the Fourier transformation of $G_{kk'}(t - t')$, then

$$G_{kk'}(t - t') = \langle\langle b_k; b_{k'}^+ \rangle\rangle = \int_{-\infty}^{\infty} G_{kk'}(\omega) e^{-i\omega(t-t')} d\omega$$

(3.52)

The delta function is defined as

$$\delta(t - t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega(t-t')} d\omega$$

(3.53)

Substituting equations (3.52) and (3.53) in to equation (3.54) we have

$$\omega G_{kk'}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega(t-t')} d\omega$$

(3.54)

The Fourier transform of equation (3.54) can be obtained by multiplying both sides by

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega_k(t-t')} dt.$$

$$\omega \int_{-\infty}^{\infty} G_{kk'}(\omega) d\omega \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(\omega-\omega_k)(t-t')} dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(\omega-\omega_k)(t-t')} dt + \langle\langle [b_k, H]; b_{k'}^+ \rangle\rangle$$

(3.55)

By using Fourier integral theorem $\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(\omega-\omega_k)(t-t')} dt = \delta(\omega - \omega_k)$

Eq. (3.55) could be written as

$$\omega G_{kk'}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \delta(\omega - \omega_k) d\omega \langle [b_k, b_{k'}^+] \rangle + \langle \langle [b_k, H]; b_{k'}^+ \rangle \rangle$$

(3.56)

From properties of Direc delta function $\int_{-\infty}^{\infty} \delta(x) dx = 1$. Therefore, for

$\omega = \omega_k, \delta(\omega - \omega_k) d\omega = 1$ more simplified form of eq. (3.56) is

$$\omega G_{kk'}(\omega) = \frac{1}{2\pi} \langle [b_k, b_{k'}^+] \rangle + \langle \langle [b_k, H]; b_{k'}^+ \rangle \rangle$$

(3.57)

$$\text{But } [b_k, H] = [b_k, \sum_k \omega_k b_{k'}^+, b_k] = \sum_{kk'} \omega_k [b_k, b_{k'}^+, b_k]$$

$$= \sum_{kk'} \omega_k [b_k, b_{k'}^+] b_k + \sum_{kk'} \omega_k b_{k'}^+ [b_k b_k] = \sum_{kk'} \omega_k b_k \delta_{kk'} + 0 = \omega_k b_k$$

where for $k = k', \delta_{kk'} = 1$

Recall the commutation and anti-commutation of operators as: for two boson operators

$$[b_k, b_{k'}^+] = b_k b_{k'}^+ + b_{k'}^+ b_k = \delta_{kk'}, \text{ and for two fermions operator } [b_k b_k] = [b_k b_{k'}^+] = 0. \text{ Eq. (3.57)}$$

becomes

$$\omega G_{kk'}(\omega) = \frac{1}{2\pi} + \langle\langle \omega_k b_k, b_k^+ \rangle\rangle$$

(3.58)

where $\langle\langle \omega_k b_k, b_k^+ \rangle\rangle = \omega_k \langle\langle b_k, b_k^+ \rangle\rangle = \omega_k G_{kk'}(\omega)$, we get eq. (3.59) as

$$(\omega - \omega_k) G_{kk'}(\omega) = \frac{1}{2\pi} \Rightarrow G_{kk'}(\omega) = \frac{1}{2\pi(\omega - \omega_k)}$$

(3.59)

The correlation function $\langle b_k, b_{k'}^+ \rangle$ is related to the analytic property of Greens function as

$$\langle b_k; b_{k'}^+ \rangle = i \int_{-\infty}^{\infty} \frac{[\langle\langle b_k, b_{k'}^+ \rangle\rangle_{\omega+i\epsilon} - \langle\langle b_k, b_{k'}^+ \rangle\rangle_{\omega-i\epsilon}] e^{-i\omega(t-t')} d\omega}{e^{\beta\omega} - 1}$$

(3.60)

Where ω_k is imaginary part of energy and ω is the real energy of Green function that have at

$$\text{pole} \frac{1}{x \pm i\epsilon} = P \frac{1}{x} \mp i\pi\delta(x)$$

$$\langle\langle b_k, b_k^+ \rangle\rangle = \frac{1}{2\pi[(\omega+i\epsilon) - \omega_k]} = \frac{1}{2\pi} \left[\frac{P}{(\omega - \omega_k)} - i\pi\delta(\omega - \omega_k) \right]$$

(3.61)

$$\langle\langle b_k, b_k^+ \rangle\rangle = \frac{1}{2\pi[(\omega-i\epsilon) - \omega_k]} = \frac{1}{2\pi} \left[\frac{P}{(\omega - \omega_k)} + i\pi\delta(\omega - \omega_k) \right]$$

(3.62)

where P is the principal part of the integral which exclude the poles. By substituting eq. (3.61) and (3.62) in to (3.60) at equal time correlation $t = t'$ we get

$$\begin{aligned}
\langle b_k, b_k^+ \rangle &= i \int_{-\infty}^{\infty} \frac{\frac{1}{2\pi} \left[\frac{P}{\omega - \omega_k} - i\pi\delta(\omega - \omega_k) \right] - \left(\frac{1}{2\pi} \left[\frac{P}{\omega - \omega_k} + i\pi\delta(\omega - \omega_k) \right] \right)}{e^{\beta\omega} - 1} d\omega \\
&= \frac{i}{2\pi} \frac{\int_{-\infty}^{\infty} [-i\pi\delta(\omega - \omega_k) - i\pi\delta(\omega - \omega_k)]}{e^{\beta\omega} - 1} d\omega \\
&= \frac{i}{2\pi} \frac{\int_{-\infty}^{\infty} [-2i\pi\delta(\omega - \omega_k)]}{e^{\beta\omega} - 1} d\omega = i \int_{-\infty}^{\infty} -i \frac{\delta(\omega - \omega_k)}{e^{\beta\omega} - 1} d\omega \\
\langle b_k, b_k^+ \rangle &= \int_{-\infty}^{\infty} \frac{\delta(\omega - \omega_k)}{e^{\beta\omega} - 1} d\omega
\end{aligned}$$

(3.63)

At $\omega = \omega_k$, $\delta(\omega - \omega_k) = 1$ otherwise zero, hence for a single mode

$$\langle b_k, b_k^+ \rangle = \frac{1}{e^{\beta\omega_k} - 1}$$

(3.64)

where $\beta = \frac{1}{K_B T}$ Hence we get,

$$\langle n_k \rangle = \frac{1}{e^{\beta\omega_k} - 1}$$

(3.65)

Where $\langle n_k \rangle = \langle b_k, b_k^+ \rangle$ is the number of magnons in state k.

3.3 Exchange Energy in DMS

Consider two interacting atoms or ions. Their resultant exchange energy is determined by the resultant spin moments of the ions S_i and S_j , if localized at sites i and j . Following Heisenberg exchange Hamiltonian such that,

$$E_{ex} = -\sum_{i \neq j} J_{ij} \langle S_i \cdot S_j \rangle \quad (3.66)$$

Where J_{ij} is an average exchange integral for the overlapping ions.

In the nearest neighbor (i.i) approximation, if the i^{th} magnetic ion interacts equally with each of Z nearest neighbors, situated at the j^{th} site with spin moments S_j , the total exchange energy is given by

$$E_{ex} = -J_{ij} \sum_j^Z \langle S_i \cdot S_j \rangle \quad (3.67)$$

Where the summation is over Z neighbors. If \mathbf{p} is the dipole moment of the Z neighbors and assuming only the spin contributes to the magnetic moments, we have:

$$P = g\mu_B \sum_j^Z S_j \quad (3.68)$$

Which gives:

$$\sum_j^Z S_j = \frac{P}{g\mu_B} \quad (3.69)$$

Where g is the lande g' -factor, which is assumed to be the same for all Z neighbors.

Substituting Eq. (3.69) into Eq. (3.67), we have,

$$E_{ex} = \frac{-J_{ij}}{g\mu_B} \langle S_i \cdot P \rangle \quad (3.70)$$

Let the magnetic moment of the i^{th} ion be,

$$\mu_i = g\mu_B S_i \quad (3.71)$$

$$\text{Hence, } S_i = \frac{\mu_i}{g\mu_B} \quad (3.72)$$

Substituting equation (3.72) in to equation (3.70),

$$E_{ex} = \frac{-J_{ij}}{(g\mu_B)^2} \langle \mu_i \cdot p \rangle \quad (3.73)$$

The intensity of magnetization \mathbf{M} , in which all N magnetic lattice points in the sample are likely to be occupied by impurity ions and is given by,

$$M = \frac{Np}{Z} \quad (3.74)$$

Where p is the average of \mathbf{p} over all groups of Z ions in unit volume.

Assuming no fluctuation of \mathbf{p} from point to point, we may replace p by \mathbf{p} and we get,

$$M = \frac{NP}{Z} \quad \text{or } P = \frac{ZM}{N} \quad (3.75)$$

$$E_{ex} = \frac{-J_{ij}}{g^2\mu_B^2} \langle \mu_i \cdot P \rangle = \frac{-ZJ_{ij}}{Ng^2\mu_B^2} \langle \mu_i \cdot M \rangle \quad (3.76)$$

Following: $E = -g\mu_B m_s H$,

$$E_{ex} = -\mu_i \cdot H_{int} \quad \text{and } H_{int} = \gamma M \quad (3.77)$$

Thus, using equation (3.77) in equation (3.76), we obtain,

$$E_{ex} = -\mu_i \gamma M = \frac{-ZJ_{ij}}{Ng^2\mu_B^2} \langle \mu_i \cdot M \rangle, \quad (3.78)$$

$$\text{Where, } \gamma = \frac{ZJ_{ij}}{Ng^2\mu_B^2} \quad (3.79)$$

Equation (3.79) refers molecular field constant.

3.4 Number of magnons in Mn-doped ZnTe DMS

A magnon is a quantized spin wave [47]. The ground state of a simple ferromagnet has all spins parallel. At long wave lengths $ka \ll 1$, so that the frequency of magnon ω_k becomes proportional to k^2 . The excitation of magnon refers to the reversal of one spin $\frac{1}{2}$. Equation (3.65) is the Bose-Einstein distribution function that magnons also obey. The total number of magnons in all modes excited at temperature T is calculated as follows,

$$\sum_k \langle n_k \rangle = \int D(\omega) n(\omega) d\omega \quad (3.80)$$

where $D(\omega)$ is the number of magnon modes per unit frequency range, $\langle n_k \rangle$ is the average number of magnons in state k and $\omega_k = 2xJSa^2k^2$ is the long wave length magnon dispersion.

At low temperature, the integral is between 0 and ∞ since $\langle n(\omega) \rangle \rightarrow 0$ exponentially as $\omega \rightarrow \infty$. Magnons are single polarization for each value of k [48].

Substituting the value at ω_k from equation (3.65), we have,

$$\langle b_k^+ b_k \rangle = \frac{1}{e^{2xJSk^2a^2/K_B T} - 1} \quad (3.81)$$

$$\sum_k \langle n_k \rangle = \frac{1}{(2\pi)^3} \int_0^\infty \frac{4\pi k^2 dk}{e^{2xJSk^2a^2/K_B T} - 1} \quad (3.82)$$

$$\sum_k \langle n_k \rangle = \frac{1}{2\pi^2} \int_0^\infty \frac{k^2 dk}{e^{2xJSk^2a^2/K_B T} - 1} \quad (3.83)$$

$$\text{Let, } y = \frac{2xJSa^2k^2}{K_B T} \quad \text{and } dy = \frac{4xJSa^2k dk}{K_B T}$$

$$\text{Solving for k, we get } k = \left(\frac{K_B T}{2xJSa^2} \right)^{1/2} y^{1/2} \quad (3.84)$$

$$\text{But } k^2 = \frac{yK_B T}{2xJSa^2}$$

$$dk = \frac{1}{2} \left(\frac{K_B T}{2xJSa^2} \right)^{1/2} y^{-1/2} dy$$

$$k^2 dk = \frac{1}{2} \left\{ \left(\frac{K_B T}{2xJSa^2} \right)^{3/2} y^{1/2} dy \right\} \quad (3.85)$$

Substituting equation (3.85) in to equation (3.83) we have,

$$\sum_k \langle n_k \rangle = \frac{1}{2\pi^2} \left(\frac{K_B T}{2xJSa^2} \right)^{3/2} \int_0^\infty \frac{y^{1/2}}{e^y - 1} dy \quad (3.86)$$

$$\text{Where the integration } \int_0^\infty \frac{y^{1/2}}{e^y - 1} dy = 2.3174$$

Therefore, we get,

$$\sum_k \langle n_k \rangle = (2.3174) \left(\frac{1}{2\pi^2} \right) \left(\frac{K_B T}{2xJSa^2} \right)^{3/2} \quad (3.87)$$

$$\sum_k \langle n_k \rangle = (0.0587) \left(\frac{K_B T}{2xJSa^2} \right)^{3/2} \quad (3.88)$$

Equation (3.88) is the average total number of magnons.

3.5 Magnetization and Temperature of Mn-doped ZnTe DMS

Temperature dependent magnetization of a ferromagnetic material at low temperature is given as,

$$M(T) = M(0) - g\mu_B \sum_k \langle n_k \rangle \quad (3.89)$$

Where $M(0) = g\mu_B N$ is the ground state magnetization at absolute zero temperature where all spins are parallel.

$$M(T) = g\mu_B nS \left(1 - \frac{1}{nS} \sum_k \langle n_k \rangle \right) \quad (3.90)$$

Substituting Eq. (3.88) in to Eq. (3.90), we obtain,

$$M(T) = g\mu_B nS \left[1 - \frac{1}{nS} (0.0587) \left(\frac{K_B T}{2xJSa^2} \right)^{3/2} \right] \quad (3.91)$$

where n is number of atoms per unit volume of lattice cell ($n = N/V = N/a^3$) and N is 1, 2, 4 for Sc, bcc and fcc lattice respectively [49]. For instance, zinc blend ZnMnTe has fcc lattice structure is given as, $\frac{4}{a^3}$. The ratio of temperature dependent magnetization M(T) and zeroth temperature magnetization M(0) gives,

$$\frac{M(T)}{M(0)} = 1 - \frac{0.0587}{4S} \left(\frac{K_B T}{2xJS} \right)^{3/2} \quad (3.92)$$

3.6 Magnon Heat capacity of Ferromagnetic Mn-doped ZnTe DMS

Magnons are another important type of energy excitation and they occur in magnetically ordered solids [50]. The internal energy of unit volume of magnon gas in thermal equilibrium at a temperature T_i neglecting magnon-magnon interaction, at very low external field and considering $ka \ll 1$ is given by:

$$U = \sum_k \omega_k \langle \tilde{n}_k \rangle_T = \sum_k \frac{\omega_k}{e^{\beta \omega_k} - 1} \quad (3.93)$$

$$\text{Taking } \omega_k = 2xJSa^2 k^2 \quad (3.94)$$

$$U = \frac{1}{(2\pi)^3} \int_0^\infty \frac{\omega_k 4\pi k^2 dk}{e^{\frac{K_B T}{2xJSa^2 k^2}} - 1} \quad (3.95)$$

$$U = \frac{1}{2\pi^2} \int_0^\infty \frac{\omega_k k^2 dk}{e^{\beta \omega_k} - 1} \quad (3.96)$$

$$U = \frac{1}{2\pi^2} \int_0^\infty \frac{2xJsa^2 k^4 dk}{e^{2xJsa^2 k^2/k_B T} - 1}, \text{ since } \beta = 1/K_B T \quad (3.97)$$

Let $y = \frac{2xJsa^2 k^2}{K_B T}$, solving for k, we get

$$k^2 = \frac{yK_B T}{2xJsa^2} \Rightarrow k = \left(\frac{yK_B T}{2xJsa^2} \right)^{1/2}, k = \frac{(yK_B T)^{1/2}}{(2xJsa^2)^{1/2}} \quad (3.98)$$

$$dk = \frac{1}{2} \frac{(K_B T)^{1/2} y^{-1/2}}{(2xJsa^2)^{1/2}} dy \quad (3.99)$$

Substituting equation (3.98) and (3.99) in to equation (3.97), we get,

$$U = \frac{(2xJsa^2)}{2\pi^2} \int_0^\infty \frac{1}{2} \frac{\frac{(yK_B T)^2 (K_B T)^{1/2} y^{-1/2}}{(2xJsa^2)^2 (2xJsa^2)^{1/2}}}{e^y - 1} dy$$

$$U = (2xJsa^2)^{-3/2} (K_B T)^{5/2} \frac{1}{4\pi^2} \int_0^\infty \frac{y^{3/2}}{e^y - 1} dy \quad (3.100)$$

Where $\frac{1}{4\pi^2} \int_0^\infty \frac{y^{3/2}}{e^y - 1} dy = 0.0456$ then, $U = 0.0456 \left(\frac{1}{2xJsa^2} \right)^{3/2} K_B^{5/2} T^{5/2}$ (3.101)

Specific heat capacity of magnons will be calculated as:

$$C^{\text{magnon}} = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T} \sum_k \omega_k \langle \tilde{n} \rangle_T \quad (3.102)$$

$$C^{\text{magnon}} = \frac{\partial}{\partial T} \left[0.0456 \left(\frac{1}{2xJsa^2} \right)^{3/2} K_B^{5/2} T^{5/2} \right] \quad (3.103)$$

$$C^{\text{magnon}} = 0.113 \left(\frac{1}{2xJsa^2} \right)^{3/2} K_B^{5/2} T^{3/2} \quad (3.104)$$

This shows that, $C^{\text{mgnon}} \sim T^{\frac{3}{2}}$

3.7 Ferromagnetic Transition Temperature of Mn-doped ZnTe DMS

The ferromagnetic transition temperature due to an indirect exchange interaction is calculated for DMS. The magnetization for density of Mn in $(\text{Zn}_{1-x}\text{Mn}_x\text{Te})$, is given by,

$$M = \frac{N_{\text{Mn}}g^2\mu_B^2}{3K_B T} S(S+1)H \quad (3.105)$$

The total effective field is the sum of the applied magnetic field (H_{app}) and the internal field (H_{int}).

$$\text{Thus, } H = H_{\text{app}} + H_{\text{int}} \quad (3.106)$$

Substituting equation (3.105) in to equation (3.106),

$$M = \frac{N_{\text{Mn}}g^2\mu_B^2}{3K_B T} S(S+1)(H_{\text{app}}+H_{\text{int}}) \quad (3.107)$$

Where $H_{\text{int}}=\gamma M$, substituting in to equation (3.107) gives

$$M = \frac{N_{\text{Mn}}g^2\mu_B^2}{3K_B T} S(S+1)(H_{\text{app}} + \gamma M) \quad (3.108)$$

The susceptibility χ is the ratio of magnetization and the applied field,

$$\chi = \frac{M}{H_{\text{app}}} = \frac{N_{\text{Mn}}g^2\mu_B^2}{3K_B T} S(S+1) \left(\frac{H_{\text{app}}}{H_{\text{app}}} + \frac{\gamma M}{H_{\text{app}}} \right) = \frac{C}{T} (1 + \gamma\chi) \quad (3.109)$$

$$\text{Where, } C = \frac{N_{\text{Mn}}g^2\mu_B^2}{3K_B} S(S+1) \quad (3.110)$$

is called Curie constant. From equation (3.109) susceptibility is

$$\chi = \frac{C}{T-\gamma C} \quad (3.111)$$

$$\text{From equation (3.111), } T_c = \gamma C \quad (3.112)$$

is the Weiss constant and it is the transition temperature T_c .

Substituting γ and C equation (3.112) becomes,

$$T_c = \frac{ZJ_{ij}}{Ng^2\mu_B^2} \frac{N_{Mn}g^2\mu_B^2}{3K_B} \quad (3.113)$$

Which can be reduced to,

$$T_c = \frac{N_{Mn}ZJ_{ij}}{3NK_B} S(S+1) \quad (3.114)$$

J_{ij} is the exchange interaction. $N_{Mn} = \frac{4}{\alpha^3} x$ is the Mn density in $Zn_{1-x}Mn_xTe$ with a lattice constant α .

The concentration of magnetic impurity is given by $x = \frac{N_{imp}}{N}$, where $N_{imp} = N_{Mn}$ is the number of impurities randomly distributed on lattice of N sites [39]. Therefore, ferromagnetic transition temperature T_c given as,

$$T_c = \frac{xZJ_{ij}}{3K_B} S(S+1) \quad (3.115)$$

CHAPTER 4

4. Results and Discussion

In chapter 3 we have expressed mathematical relations of magnetization, transition temperature for ferromagnetic DMS and specific heat capacity of magnons based on spin wave using Holstein-Primakoff transformations. We have also calculated the average number of magnons excited at T in k mode using the Green function. We have described dispersion relation for magnons in ferromagnetic DMS which is quadratic in k. The dispersion relation of magnons is used to calculate all other quantities stated above.

In this chapter, we will present the main results obtained in this work and also investigate those using figures.

4.1 Number of magnons and temperature for Mn-doped ZnTe DMS

The average number of magnon as a function of temperature is plotted below according to equation (3.88).

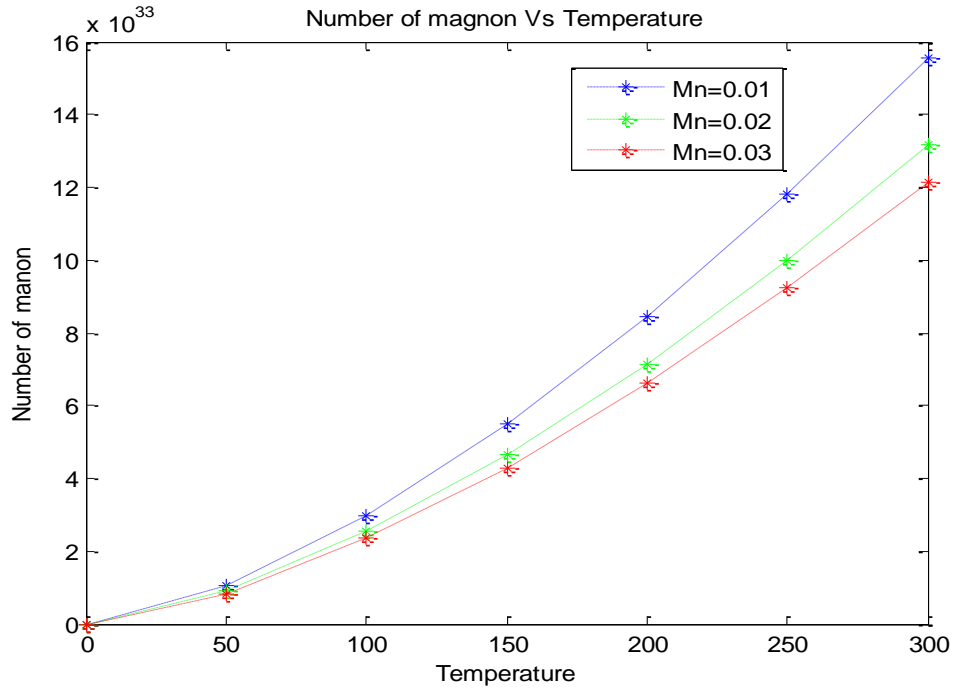


Figure 4.1 Number of magnon versus temperature for $x = 0.01$.

Using constants for $Zn_{1-x}Mn_xO, \alpha = 3.25 \text{ \AA}, J = 2 \times 10^{-23} \text{ Joules}, S = \frac{5}{2}, K_B = 1.38 \times 10^{-23} \text{ J/K}, x = 0.01$, we have obtained the total number of magnons. Number of magnons and temperature have linear (direct) ($\langle n_k \rangle \sim T^3$), relationship. Generally, we can understand that increasing temperature increases the number of magnons.

4.2 Magnetization and Temperature in Mn-doped ZnTe DMS

The reduced magnetization as a function of temperature can be described using each spin-wave excitation. Mathematically, temperature dependent magnetization is written as given in equation (3.92),

Using the above relation, we can relate them graphically as follows,

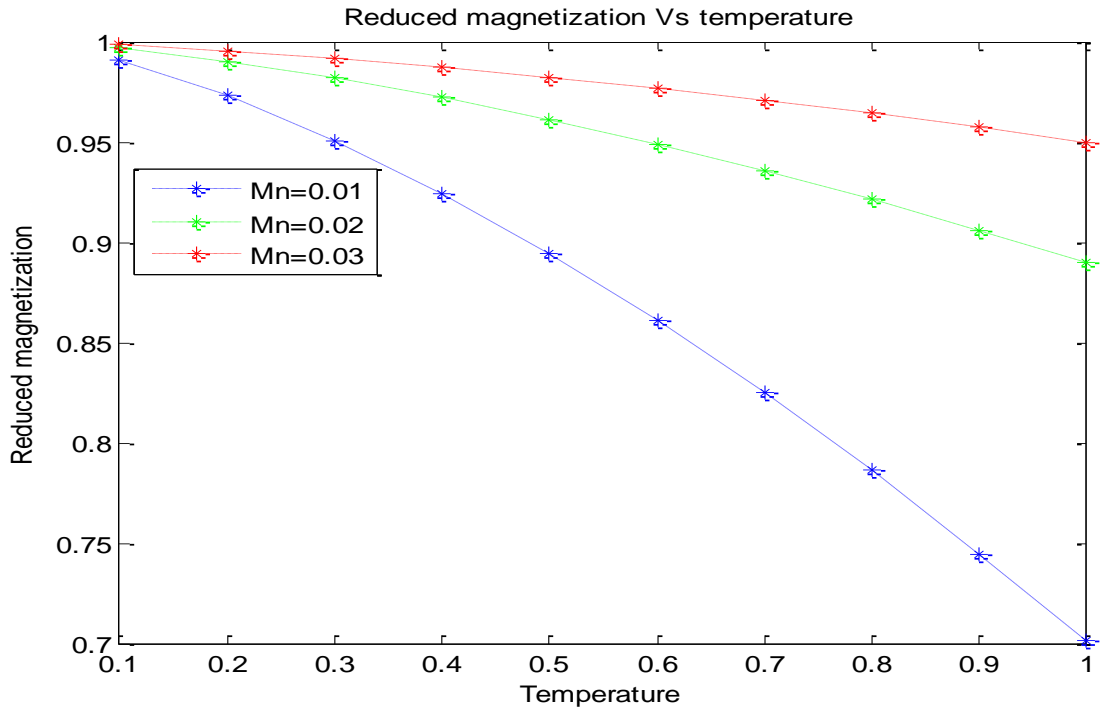


Figure 4.2 Reduced magnetization versus temperature for $x = 0.01$.

As can be seen from Figure 4.2 magnetization decreases as temperature increases. The calculated curve fits to the experimental results obtained by C.Marino et al., 2000 [51].

4.3 Transition temperature and concentration in Mn-doped ZnTe DMS

The concentration of the magnetic impurity x is linearly related to the ferromagnetic transition temperature T_c as shown in equation (3.113).

Following the above equation we can plot the graph of transition temperature versus concentration as follows,

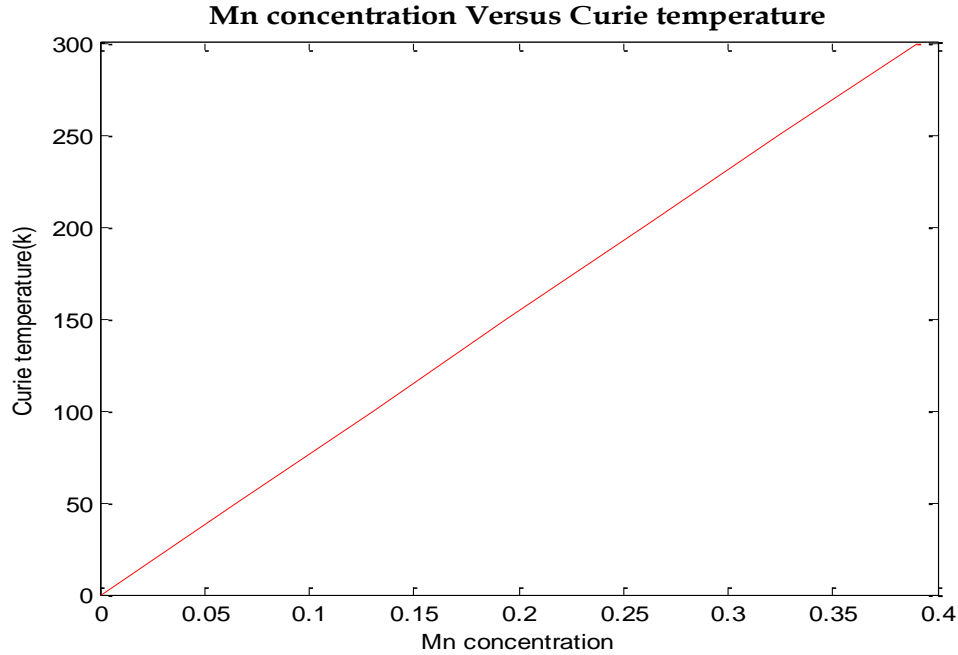


Figure 4.3 linear dependence of T with Manganese concentration

As can be seen from Figure 4.3, there is direct proportionality relation between Curie temperature T_c and impurity concentration x . As the concentration of dopant increases temperature also increases. The calculated curve fits to the experimental result obtained by Matsukura et al. [52].

4.4 Magnon Specific heat capacity and temperature for Mn-doped ZnTe DMS

Magnon specific heat capacity versus temperature for ferromagnetic ZnMnTe is shown mathematically in this work. Specific heat capacity of magnon is expressed in equation (3.104).

Using equation (3.104), the graph of magnon specific heat capacity versus temperature is plotted as shown in Figure 4.4.

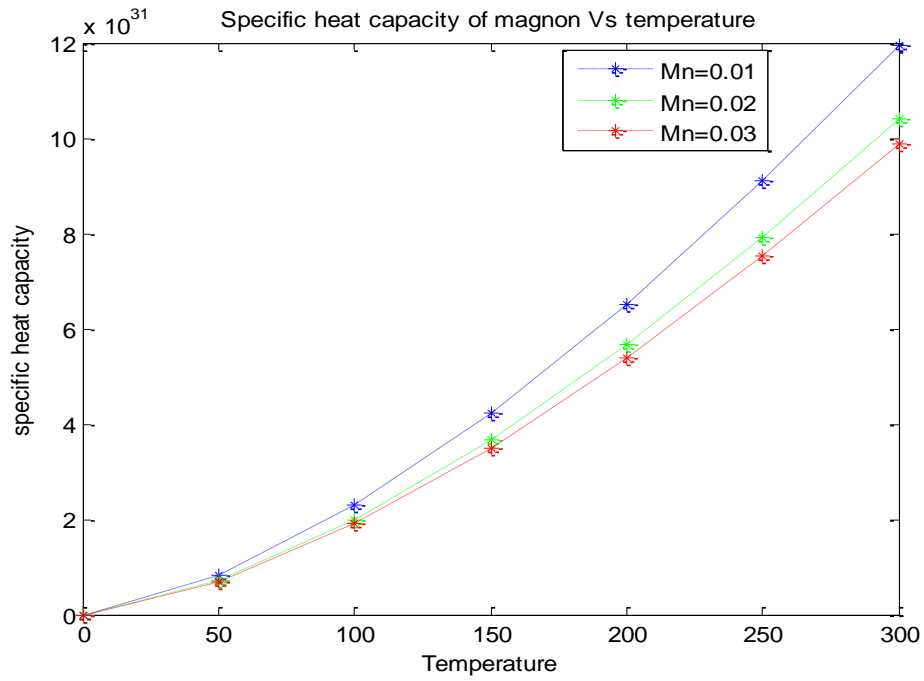


Figure 4.4 Magnon specific heat capacity vs temperature for $x = 0.01$

As can be seen from Figure 4.4 the specific heat capacity of magnon increases with increase of temperature. The calculated curve fits to the experimental result obtained by Jurgen Konig et al. [53].

CHAPTER FIVE

5. Conclusion and Recommendations

The main objective of this work is to study ferromagnetism in Mn-doped ZnTe DMS. From the previous chapter, we have expressed different quantities of the system mathematically using Green function formalism. The average number of magnons and specific heat capacity of magnons depends on temperature with relation $T^{3/2}$. As the temperature increases the number of magnon excitation increases. The transition temperature depends on the concentration of manganese impurity and have direct relation. We conclude that magnetization decreases with increasing temperature. The magnon dispersion in ferromagnetic DMS has the $\omega_k = AK^2$ relation which is parabolic wave vector dispersion. We can also conclude that ferromagnetic transition temperature of ZnMnTe DMS linearly depends on concentration of manganese impurity. The number of magnons increases due to the increase of temperature but decreases with magnetization.

The recommendation based on the study results that: recently, Mn-doped ZnTe DMSs have been widely studied materials. Compare to all other DMSs, these materials have numerous advantages for applications of modern technological spintronic devices. Room temperature ferromagnetism is an important property for applications of spintronic devices. However, origin and mechanism of ferromagnetic behavior in these DMSs are still controversial and debatable. It requires more precise study for the origin of ferromagnetism on Mn-doped ZnTe DMS for future research.

References

- [1] S.M.SZE.M.K.LEE, (2010), Semiconductor devices physics and Technology, 3rd ed., John Wiley and Sons.Inc.
- [2] Dietl, T., Ohno, H., Matsukura, F., Cibert, J., and Ferrand, D. (2000) Zener Model Description of Ferromagnetism in Zinc-Blend Magnetic semiconductors. Science, 287, 1019-1022.
- [3] Gibbon,P.Mash-Free Simulation of high intensity laser interaction with collisional plasmas. In NIC Symposium 2006 (pp.333-340).
- [4] C. Kittel, (1986), Introduction to Solid State Physics, 6thed (John Wiley and sons,New York).
- [5] D. A. NEAMEN, (1992), Semiconductor Physics and Devices: Basic principles, (Richard D. Irwin, INC., University of New Mexico).
- [6] C. Timm, (2003), “Disorder effects in diluted magnetic semiconductors”, J. Phys: Condens. Matter 15, R1865
- [7] C. Chappert, C., Fert, A., and F. N. Van Dau, F. N. (2007) The emergence of spin electronics in data storage. Nat. Mater. 6, 813-823.
- [8] Liu C., Yun F., Morkoc H., (2005). Ferromagnetism of ZnO and GaN: A review Journal of Materials Science: Materials in Electronics, 16(9), 555.
- [9] Sharma P, Gupta A, Rao K V, Owens F J, Sharma R, Ahuja R, Osro J M Guillen, Johansson B, Gehring G A (2003) Nature Materials 2 673
- [10] C.Amente, (2010), PhD dissertation, Addis Ababa University, Study of photoinduced FM in DMS (Ga,Mn)As
- [11] B. T. Matthias, R. M. Bozorth, and J. H. Van Vleck, (1961) Ferromagnetic interaction in EuO. Physical Review Letters 7, 160.
- [12] Mauger, A., and Godart, C. (1986). The magnetic, optical, and transport properties of representatives of a class of magnetic semiconductors: The europium Chalcogenides. Physics Reports, 141(2-3), 51-176.

- [13] Norasetthekul, S., Park, P. Y., Baik, K. H., Lee, K. P., Shin, J. H., Jeong, B. S., ... & Pearton, S.J. (2001). Dry etch Chemistries for TiO_2 thin films. *Applied surface Science*, 185(1-2), 27-33.
- [14] K. Khazen (2008). Phd. Desseration in Ferromagnetic reason once Investigation of GaMnAs Nanometric layers.
- [15] J. Mahanty, (1974). *The Green function method in Solid State Physics*, East-WestPress, New Delhi.
- [16] Bergqvist, L., Eriksson, O., Kudrnovsky J., Drchal, V., Korzhavyi, P., & Turek, I. (2004). Magnetic percolation in diluted semiconductors. *Physical Review Letters*, 93(13), 137202.
- [17] J. A Gaj, J. Kossut, (2010) spring series in material science. 144, 1007.
- [18] Mizokawa, T., Nambu, T., Fujimori, A., Fukumura, T., &Kawasaki, M. (2002).Electronic structure of the oxide-diluted magnetic semiconductor $Zn_{1-x}Mn_xO$. *Physical Review B*, 65(8), 085209.
- [19] Chen, Y. F., Huang, J. H., Lee, W. N., Chin, T. S., Huang, R. T., Chen, F. R., ... & Ku, H. C. (2007). Room-temperature ferromagnetism in self-assembled (In, Mn) As quantum dots. *Applied Physics letters*, 90(2), 022505.
- [20] Reynolds D.C., Look D.C., Jogai B., Litton C.W., Cantwell G., and Harsch W.C., (2003). A comprehensive review of ZnO materials and devices.
- [21] Turner A. E., Gunshor R. L., and Datta S., (1988), New class of materials for optical isolators, *Appl. Optics*, 22, 3252.
- [22] Kaldis E., (1981), *Current Topics in Materials Science*, North-Holland Publishing Company.
- [23] Kim, H., Vogelgesang, R., Ramdas, A. K., Peiris, F. C., Bindley, U., &Furdyna, J.K. (1988). MnSe: Rocksalt versus Zinc-blend structure. *Physical Review B*, 58(11), 6700.
- [24] Singhal R. K., Sharma S. C., Kumari P., Sudhish Kumar, Xing Y. T., Deshpande U. P., Shripathi T., and Elisa Saitovitch, (2011) *Journal of Applied Physics*, 109, 063907

- [25] Shanon R. (1976), "Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides." *Acta Crystallographica Section A*. 751-767.
- [26] Blythe, H. J., Ibrahim, R. M., Gehring, G. A., Neal, J. R., Fox, A. M. (2004). "Mechanical alloying: a route to room-temperature ferromagnetism in bulk $Zn_{1-x}Mn_xO$. *Journal of magnetism and magnetic materials*, 283 (1), 117-127.
- [27] Kane, M. H., Shalini K., Summers, C. J., Vartharajan, R., Nause, J., Vestal, C. R.,...& Ferguson, I. T. (2005). Magnetic properties of bulk $Zn_{1-x}Mn_xO$ and $Zn_{1-x}Mn_xO$ single crystals. *Journal of applied Physics*, 97(2)023906.
- [28] Kittiertuilstved, K. R., Norberg, N. S., & Gamelin, D. R. (2005). Chemical manipulation of high-Tc ferromagnetism in ZnO diluted magnetic semiconductors. *Physical Review Letters* 94(14), 147209
- [29] Pradhan, A.K., K. Zhang, S. Mohanty, J.B. Dadson, D. Hunter, J. Zhanga et al. (2005) "High temperature ferromagnetism in pulsed-laser deposited epitaxial (Zn,Mn) thin films: Effects of substrate temperature." *Applied Physics Letters* 86 152511.
- [30] Sheaba, R.A.J., Saravanakmar, S., Israel, S., & Saravanan, R. (2017). Understanding electronic and magnetic transition ball milled diluted magnetic semiconductor $Si_{1-x}Ni_x$ through experimental density distribution. *Journal of Alloys and compounds*, 728, 887895.
- [31] S. J. Ward, (1995). *Compound semiconductor device physics*, 3rd ed., Walter Meibner institut.
- [32] Tsuruoka, J., Tamimoto, R., Tachikawa, N., Ushio, S., Matsukura, F., & Ohno, H. (2002). Microscopic identification of dopant atoms in Mn-doped GaAs layers. *Solid state communications*, 121 (2-3), 79-82.
- [33] Fert, A., & Campbell, I. A. (1976). Electrical resistivity of ferromagnetic nickel and iron based alloys. *Journal of Physics F: Metal Physics*, 6(5), 849.

- [34] B. Belhadji (2008), Ph.D dissertation, Forschungszentrum Julich, Germany.
- [35] Nan Zheng, (2008) Introduction to Dilute Magnetic Semiconductors, department of Physics and Astronomy, The University of Tennessee Knoxville Dated: April 13, USA.
- [36] Schwabe N. F., Elliott R. J., and Wingreen N. S., (1996), Ruderman-Kittel-Kasuya- Yosida interaction across a tunneling junction out of equilibrium, Phys. Rev. B, 54, 12953.
- [37] Yosida K., (1996), Theory of magnetism, Springer, Berlin.
- [38] Fukuma Y., Odawara F., Asada H., and Koyanagi T., (2008), Effects of annealing and chemical doping on magnetic properties in Co-doped ZnO films, Phys. Rev. B, 78, 104417.
- [39] Parkinson J.B. (1969). Phase transitions in the Spin-half $J_1 - J_2$ model. Physical Review B, 58(10), 6394.
- [40] Parkin, S.S. (2004, December). Spintronic materials and Devices., Past, present and future! In Ied M Technical Digest. IEEE international electron devices Meeting,(pp.903-906).
- [41] S. Balmukund Rahi and P. Rastogi, (2013), Introduction to Journal of Advanced in Engineering and Technology 6, 696
- [42] K. Sato, T. Ishi bashi, K. Minami, H. Yuasa, J. Jogo, T. Nagatsuka, A. Mizusawa, Y. Kangawa a and A. Koukitu (2005) J. of physics and chemistry of solid 66, 2030.
- [43] P.L. Taylor and O. Heinonen. (2002) A Quantum Approach to condensed Matter Physics. Cambridge University Press, ISBN 0521778271, UK.
- [44] M. Nolting, (2009). Fundamentals of many body physics, Verlag Berlin Heidelberg.
- [45] T. Heinzl, (2007). Mesoscopic Electronics in Solid State Nanostructure, 2nd ed., Wiley-Vch and Co.Kga.
- [46] N. Ba an and L. T. Tuong, (1991) Solid state communication. 80, 479
- [47] Hannes Raebiger, (2006), Ferromagnetism In (Ga,Mn)As And (Ga,Mn)N, Auditorium E at Helsinki University of Technology (Espoo, finland) on the 21st of April.

- [48] Shivaraman Ramachandran, (2006), PhD dissertation Zinc Oxide based Diluted Magnetic Semiconductors,
- [49] Hu, X., & Sarma, S.D (2001). Spin based quantum computation in multielectron quantum dots. Physical Review A, 64(4), 042312.
- [50] James D. Patterson Bernard C. Bailey, (2005) Solid-State Physics Introduction to the theory.
- [51] Marino, E.C., & Neto, M.B.S. (2000). Effective sublattice magnetization and Neel temperature in quantum antiferromagnets.” Physical Review B 62 No. 1. 142
- [52] Matsukura, F., Ohno, H., Shen, A., and Sugawara, Y. (1998). Transport properties and origin of ferromagnetism in (Ga,Mn)AS. Physical Review B, 57(4), R2037.
- [53] König, J., Lin, H. H., and MacDonald, A.H. (2000). Theory of diluted magnetic semiconductor ferromagnetism. Physical Review Letters, 84(24), 5628.